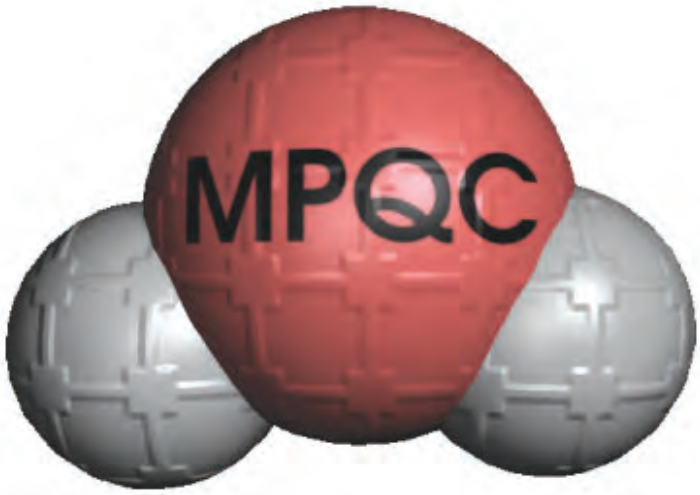
MPQC: The Massively Parallel Quantum Chemistry Program



The Massively Parallel Quantum Chemistry (MPQC) Program computes properties of atoms and molecules from first principles using the time independent Schrödinger equation. It runs on a wide range of architectures ranging from individual workstations to symmetric multiprocessors to massively parallel computers. The design is object-oriented, using the C++ programming language.

Truly quantitative chemical modeling, as well as even qualitative prediction of properties relying on electronic or nuclear effects (visible/UV absorption, NMR chemical shifts, etc.), requires quantum mechanics. Quantum chemical methods are computationally expensive; their applicability traditionally has been limited to small molecules. Developers of the MPQC package are working on several fronts to extend the range of molecules to which such methods can be applied. This work includes reducing the time to solution by efficient parallelization and improved algorithms. MPQC is designed in a modular fashion, allowing easy extension and interfacing with other software.

Unique among quantum chemistry packages, MPQC is open-source, object-oriented in design and implementation, and written from the beginning to run in parallel. Complementary to the design and implementation of reliable parallel implementations, MPQC researchers are developing reduced-scaling correlated methods that circumvent nonphysical high-order scaling with respect to molecular size. In addition, recently added state-of-the-art explicitly correlated methods are enabling extreme accuracy.

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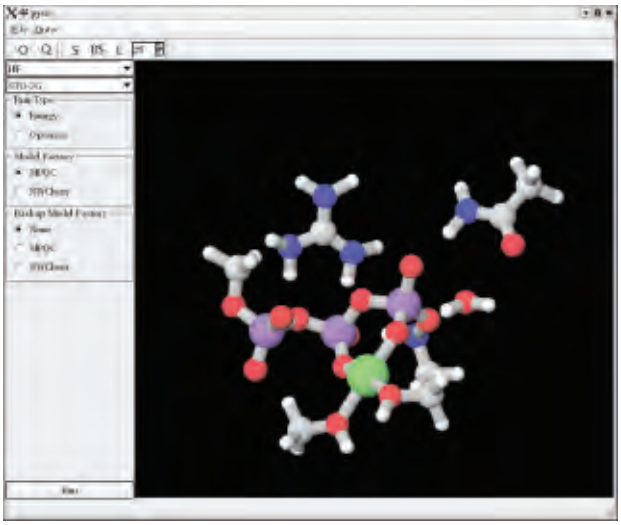


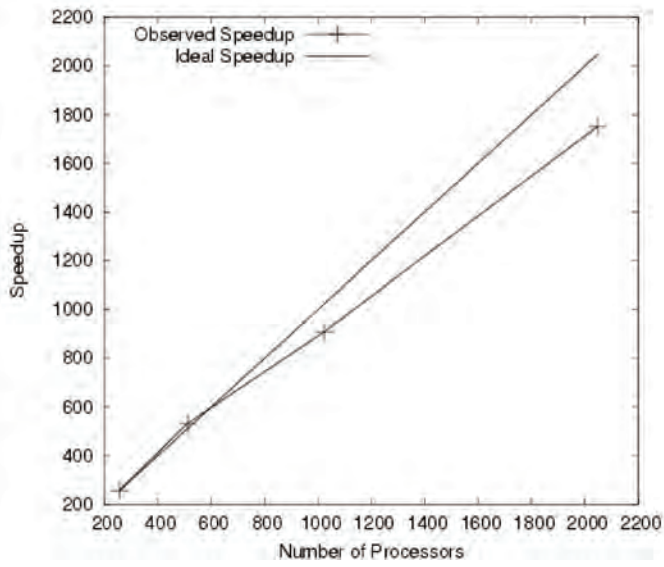
A graphical interface permitting selection of quantum chemistry packages using the CCA.

MPQC Promotes Software Interoperability via a Flexible, Adaptable Design

MPQC researchers are at the forefront of scientific software engineering. Through participation in the Common Component Architecture (CCA), standardized interfaces are being developed to promote interoperability between quantum chemistry packages and a community-based software development effort. MPQC's object-oriented approach has proven useful for managing complexity and enabling extensibility. MPQC's well-designed class hierarchy enables easy adaptation. Open source licensing encourages the reuse of existing code and allows outside researchers to examine code in detail, permitting greater return on public investment.

MPQC Runs Efficiently on Massively Parallel Computers

To obtain the full benefit from parallel machines it is important to parallelize a code from its conception. MPQC supports parallelism through three separate abstractions: message groups, thread groups, and memory groups. This provides the most appropriate and efficient model for different tasks and allows hybrid parallelization schemes to take full advantage of machine architectures.



Speed (relative to 256 processors) for computation of the uracil dimer MP2 energy on ASC White.

The Scalable Computing Research and Development Department's InfiniBand testbed.

MPQC Drives Software and Hardware Research

Developed largely within Sandia's Scalable Computing Research and Development Department, MPQC presents real world challenges for the department's vertically integrated research team. As a demanding application leveraging a range of technologies, the package drives research in parallel algorithm development, computer architecture design and evaluation, system software and middleware, performance tuning and analysis, and storage systems.

Visit the MPQC homepage at http://www.mpqc.org

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